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6. AUTHOR(S)
John R. Sabin and
Samuel B. Trickey

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Florida
Quantum Theory Project
355 Williamson Hall, P.O. Box 118435
Gainesville, FL. 32611-8435

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13. ABSTRACT (*Maximum 200 words*)

Our previous work emphasized energy deposition in ultra-thin films in the projectile energy regime near and above the stopping maximum. Not only are most stopping measurements done in that regime, but the theory is simplified under this assumption, since Bethe stopping is dominant. Thus, we have developed, demonstrated the effectiveness, and applied an approximate model which works well in this energy domain. We have predicted a number of ultra-thin film effects which await experimental verfication and technological exploitation.

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Theoretical and Numerical Prediction of Stopping Properties of Counterpart Thin Films and Solids

Final Report

John R. Sabin, P.I.

Samuel B. Trickey, Co-P.I.

May 30, 1995

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1. Statement of the Problem

Our previous work emphasized energy deposition in ultra-thin films in the projectile energy regime near and above the stopping maximum. Not only are most stopping measurements done in that regime, but the theory is simplified under this assumption, since Bethe stopping is dominant. Thus, we have developed, demonstrated the effectiveness, and applied an approximate model which works well in this energy domain. We have predicted a number of ultra-thin film effects which await experimental verification and technological exploitation.

Recently the technological challenge has shifted from high-energy projectiles (e.g. weapons effects) to lower energy exposures characteristic of such diverse environments as ion-implantation apparatus and satellite–mounted electronics. In such environments, the combination of ultra-thin materials films and low projectile energies is relatively unexplored. As we show below, we have most of the tools and techniques which need to be combined to address that family of important problems.

To give but one of several possible examples, large fluxes of low-energy ions and thin film technology have come together as a challenge to providing stable micro-electronic components in satellites and space vehicles. Although not as big a problem for now in large, earth-bound machines (in which redundancy and both hard and software bitchecking are normal since mass and volume are not such critical engineering limitations), issues of single-event upsets are a concern for weight-limited devices in high flux, but relatively low energy, radiation fields such as occur when electronics are flown. *Such problems become more severe inversely with system size.* Similarly, thin film technology has improved dramatically in recent years. It is now possible to make free-standing films (not overlayers!) routinely on the order of 25 Å. Such films, of the order of ten monolayers (*e.g.* carbon), may be supported on a macroscopic grid, but are, for all intents and purposes, free standing.

2. Summary of Results

Progress and accomplishments during 1991–95 (first half) are conveniently divided into four categories:

1. Conception, implementation, testing and first applications of the **CHANNEL** code,
2. Continued development of the **FILMS** and **FILMSTOP** codes and their application to studies of the electronic structure and stopping properties of significant thin film systems,
3. Study and calculation of the stopping properties of several important molecular systems, and
4. implementation of the generalized oscillator strength (GOS) formulation of the first Born approximation stopping, with demonstration of the severity of the current practical limits on state-of-the-art, fully *ab initio* GOS calculations.

Papers cited in this section are listed in the section headed "Papers Acknowledging Support from the Present Contract Period." We consider each of the four topics briefly.

1. Perhaps the most dramatic advance has taken place over the past two years, in which we have worked out the theory, design, and coding of the program **CHANNEL**, which calculates trajectories for low energy ions, $E \approx 25\ keV$, in bulk solids. The simulation relies upon

realistic, quantum mechanically derived charge densities, potentials, and dissipative forces in describing the interaction of the projectile (thus far restricted to protons) with the bulk solid target. As described in detail below, **CHANNEL** solves the classical equations of motion for the projectile in the solid. The solution enables prediction of the penetration depths and range straggling (ion implantation profiles) as well as observation of the channeling behavior of the incident ions.

The design assumptions of the code are intended to yield better (in the sense of including more of the essential physics) results than previous codes such as the Monte Carlo codes, **MARLOWE, TRIM, BCCRY, PEPPER, BABOUM** and **LAROSE**. In particular these tend to treat the scattering of the incident ions by the crystal lattice as binary collisions using screened atomic-like potentials. The dissipation force used includes, in an approximate way, both electronic and nuclear energy dissipation terms. Some programs, such as **TRIM** and **BABOUM**, treat the target as an amorphous or random solid. However, **TRIM** can do calculations of various compounds which have up to 3 layers of differing materials.

CHANNEL appears to be the first code which uses a potential and charge density generated from a quantum mechanical crystalline calculation. To keep simulation times within reason, the calculation of ion implantation profiles must be for ions of relatively modest incident energy (of the order tens of keV) simply to allow the ion to be trapped in the target within some reasonable distance. Thus, by the nature of the problem, the ion's trajectory will be influenced strongly by the potential with which it interacts. This means that a method for calculating accurate ion implantation profiles must have a very realistic representation of the crystalline potential as well as the dissipative force. The dissipation function developed by Echenique *et al.* which we use, is particularly suited for low energy ions. It expresses the energy dissipation term as a function of the local electronic density, hence allows realistic determination of the dissipative force from the solid's electronic charge density.

Testing the code involved examining protons channeling in simple cubic hydrogen, a particularly instructive and transparent case since the channel geometry (symmetry) is such that one can check the results for reasonableness by inspection and hand calculation. After debugging, we generated hypothetical ion implantation profiles for protons in the <100> channel. (Experimental data on solid atomic H are, of course, unavailable.)

A more realistic and technologically interesting case is protons in silicon. We simulated the implantation profiles of low energy protons in the <110> and <100> channels of Si in the diamond structure [space group Fd3m-O_h^7, diamond Si]. Although the calculations are expensive in terms of computer time (the program is yet to be optimized), the preliminary results are very encouraging. To determine a well-defined average penetration depth would require more trajectories, but it appears that a reasonable average depth is emerging. The results also indicate that the range in the <110> channel should be nearly 3 times that in <100>, as shown in Figure 1.

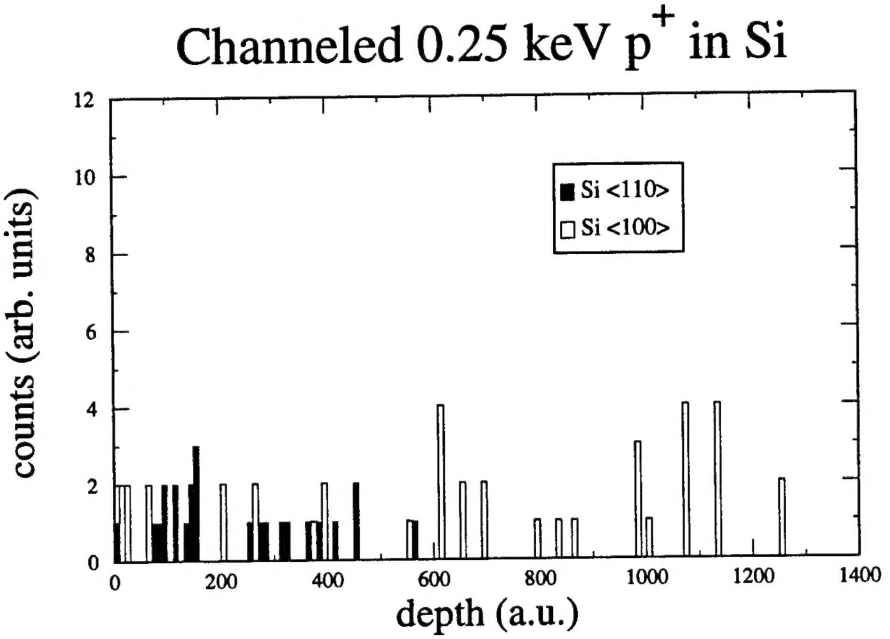

Figure 1: Deposition profiles for 0.25 keV protons in the <110> (open) and <100> (filled) channels of diamond Si

Clearly the method has great promise for predicting and interpreting the channeling behavior of low energy ions (E in the tens of keV) in extended systems. These results are new enough that they have not been published yet, but a preliminary version of the channeling of protons in hydrogen in the simple cubic structure (scH) has been submitted (paper #19).

2. The second major accomplishment was the use of the **FILMS** and **FILMSTOP** codes for large-scale study of the electronic structure and stopping of several ultrathin films. Although there were improvements in both the theory (paper #12) and fundamental interpretation (paper #16) of stopping of ultrathin films in general, the most progress by far was in predictive study of specific, paradigmatic systems.

   Quantum size effects and the dramatic distinction between bulk and ultra-thin stopping in metal films were shown in the work on Li n-layers (paper #11). In particular, there is extremely slow convergence (with increasing n) of the n-layer value of a property towards the bulk crystal value. In Li it appears that about 20 layers is needed to reach the bulk limit.

   We also treated the effects of molecular vs. atomic-like ordering upon proton stopping in a large range of H n-layers (papers #5 and 7).

   The archetypical ionic solid, LiF was studied in papers #13, 17, and 22. In the latter we showed that the 1–layer is an *indirect* gap material, in marked contrast with the crystal. Paper #13 treated the stopping at zero intraplanar strain, while #22 showed, surprisingly, that ionic 1–L stopping is so dominated by ionic binding that no qualitative change occurs for strains even as large as needed to attain gap closure and metallization.

A study of stopping in the graphite and diamond n–layers (paper #18) showed that the ratio of stopping for n-layers of the two C allotropes differs from the bulk ratio up through n = 4 at least, once again demonstrating the critical importance of multiple length scales.

3. Calculation of the stopping and electronic properties of molecules continued, with particular emphasis on the variation of those properties with molecular geometry and with orientation.

   From the directional dependence of the dipole oscillator strength distribution (DOSD), we showed (papers #2, 3, 4 and 9) that the stopping of protons of energies above 100 keV is dependent on the orientation of the target molecule. This behavior could be of use in films and bulk as well, and, perhaps, gives a clue for intrepreting the ordering of stopping in certain hydrogen films (paper #5). In addition, the geometric dependence of the mean excitation energy can be related to temperature and isotope effects (papers #14 and 21), both of which are small in molecules, the latter being only a small fraction of the former. We would expect that the same would hold in thin films and in bulk targets.

4. In an effort to move toward absolutely first-principles calculation of stopping and other energy deposition phenomena, we have attempted first Born approximation stopping calculations for some small atoms directly from the generalized oscillator strength distribution (GOSD). The procedure is to generate the GOSD for the atom directly from the polarization propagator, then obtain the stopping directly by integration of the GOSD (papers #8 and 23). The outcome is in fact an illustration of the current state of the art: the scheme can be made to work for He but not for Be.

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3. Scientific Personnel

Principal investigators

1. John R. Sabin
2. Samuel B. Trickey

Postdoctoral associates

1. Jan Nobel
2. Jin-Zhong Wu

Visitors

1. John Boettger
2. Geerd H.F. Diercksen
3. Jan Geertsen
4. Jens Oddershede